

Charge-localization and isospin-blockade in vertical double quantum dots

David Jacob

*Departamento de Física Aplicada , Universidad de Alicante,
San Vicente del Raspeig, 03690 Alicante, Spain**

Bernhard Wunsch and Daniela Pfannkuche

*I. Institute of Theoretical Physics, University of Hamburg,
Jungiusstr. 9, D-20355 Hamburg, Germany*

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Abstract

Charge localization seems unlikely to occur in two vertically coupled symmetric quantum dots even if a small bias voltage breaks the exact isospin-symmetry of the system. However for a three-electron double quantum dot we find a strong localization of charges at certain vertically applied magnetic fields. The charge localization is directly connected to new ground state transitions between eigenstates differing only in parity. The transitions are driven by magnetic field dependent Coulomb correlations between the electrons and give rise to strong isospin blockade signatures in transport through the double dot system.

Quantum dot structures are excellent systems to investigate few and many particle physics [1, 2, 3], due to the high experimental control over the system parameters. In this context double quantum dots are particularly interesting in two different manners: as an implementation of quantum bits (qubit) [4, 5] and as a model system for molecular binding under controlled conditions [3, 6, 7, 8].

In this letter we describe a new correlation effect in a vertically coupled double quantum dot (DQD) in a perpendicular magnetic field, which strongly changes the molecular binding and at the same time, defines a two level system, that can be manipulated in a controlled way and could serve as a qubit. This effect is manifest in the energy spectrum and the transport properties of the DQD. Sweeping the magnetic field we find ground state crossings in a perfectly symmetric DQD containing three electrons which – in contrast to the well known crossings between states that differ in angular momentum and/or spin [9] – occur between states with same spin and angular momentum. In contrast to a crossing between states that differ in angular momentum and/or spin, that affects the lateral motion and occurs in single dots already, the crossing discussed here involves a transition in the parity of ground state, that characterizes the vertical degree of freedom. Therefore by slightly breaking the symmetry between the two dots, e.g. by applying an infinitesimally small voltage, the crossing turns into an anticrossing, resulting in charge localization. Due to the charge localization, transport through the DQD is strongly suppressed at the anticrossing. Reducing the vertical degree of motion to an additional spin like degree of freedom, the isospin, the strong suppression of transport can be explained by an isospin blockade at the anticrossing in analogy to the well known spin blockade [10].

We describe the DQD within the layer model [9, 11], that is applicable, if the external potentials separate in a strong vertical and a considerably weaker lateral component. We assume the in-plane confinement for the electrons to be parabolic and circular symmetric. Additionally a magnetic field B can be applied in the vertical direction. The in-plane motion of the electrons is then described in the effective mass approximation by the Fock-Darwin-Hamiltonian \hat{H}_{FD} [12] and the Zeeman term \hat{H}_Z .

$$\hat{H}_{FD} + \hat{H}_Z = \frac{1}{2m^*} \left(\vec{p} + e\vec{A} \right)^2 + \frac{m^*\omega_0^2}{2} r^2 + g^* \frac{\mu_B}{\hbar} B \hat{S}_z \quad (1)$$

where ω_0 is the strength of the parabolic confinement potential, m^* is the effective mass, μ_B the Bohr Magneton and g^* the effective Landé factor [13]. The eigenstates of the in-plane

motion are the Fock-Darwin states $|n, m\rangle$ with the principal quantum number $n \in \mathbb{N}$ and the angular momentum quantum number (z -component) $m \in \mathbb{Z}$. The Hamiltonian (1) conserves the angular momentum \hat{L}_z as well as the z -component of the spin \hat{S}_z and the square of the spin \hat{S}^2 , described by m , s_z and s respectively.

The vertical motion is reduced to tunneling between two δ -sheets, labeled by the quantum number $\alpha \in \{+, -\}$. $\alpha = \pm$ corresponds to the upper dot (+) or lower dot (-) respectively. In analogy with the real electron spin one can define a spin operator algebra, where the z -component of the isospin, \hat{I}_z is given by α [11].

The interdot tunneling \hat{H}_T $|\pm\rangle = t |\mp\rangle$ which transfers electrons between the two dots can be expressed by isospin operators:

$$\hat{H}_T = t \left(\hat{I}_+ + \hat{I}_- \right) = 2t \hat{I}_x \quad (2)$$

with the real hopping parameter $t < 0$ [9]. \hat{I}_\pm are the raising and lowering operators for the z -component of the isospin, and \hat{I}_x is its x -component. The eigenstates of \hat{I}_x and thus of \hat{H}_T are the symmetric and antisymmetric linear combinations of the isospin eigenstates $|\pm\rangle$. Due to tunneling the electrons are delocalized and the eigenstates of the Hamiltonian $\hat{H}_{FD} + \hat{H}_T + \hat{H}_Z$ are no longer eigenstates of I_z . However in case of symmetric dots the two layers are identical, so that the isospin-parity \hat{P} is conserved. In case of more than one electron inside the DQD, Coulomb interaction $\hat{\mathcal{V}}_c$ between the electrons has to be included such that the few-electron Hamiltonian reads:

$$\begin{aligned} \hat{\mathcal{H}} &= \hat{\mathcal{H}}_{FD} + \hat{\mathcal{H}}_T + \hat{\mathcal{H}}_Z + \hat{\mathcal{V}}_c \\ &= \sum_{i=1}^{N_e} \left(\hat{H}_{FD}^{(i)} + \hat{H}_T^{(i)} + \hat{H}_Z^{(i)} \right) + \frac{e^2}{4\pi\epsilon\epsilon_0} \sum_{i < j} \hat{V}_c^{(i,j)}. \end{aligned} \quad (3)$$

Since Coulomb interaction is invariant under spatial and spin rotations, total angular momentum $\hat{\mathcal{L}}_z$ and total spin $\hat{\mathcal{S}}^2, \hat{\mathcal{S}}_z$ are still conserved and are described by the quantum numbers M and S, S_z respectively. For a symmetric DQD also the parity of the few electron eigenstates $\hat{P} = 2^{N_e} \cdot \hat{I}_x^{(1)} \otimes \dots \otimes \hat{I}_x^{(N_e)}$ is conserved, described by the quantum number $P \in \{+1, -1\}$. Due to Coulomb interaction the electrons are correlated. In a vertical double quantum dot the Coulomb interaction can be divided into two parts: $\hat{V}_c^{(i,j)} = \hat{V}_{intra}^{(i,j)} + \hat{V}_{inter}^{(i,j)}$. The *intradot* Coulomb interaction $\hat{V}_{intra}^{(i,j)} = 1/r_{ij}$ describes the interaction between electrons localized in the same dot, whereas the *interdot* Coulomb interaction $\hat{V}_{inter}^{(i,j)} = 1/(r_{ij}^2 + d^2)^{1/2}$

describes the interaction between electrons localized in different dots. Here $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the lateral separation of two electrons i and j and d is the vertical separation between the dots. The Coulomb operator commutes with the z -component of the total isospin $\hat{\mathcal{I}}_z$ but does not commute with $\hat{\mathcal{I}}_x$ and accordingly $\hat{\mathcal{H}}_T$. The commutator between Coulomb interaction and tunneling depends on the difference between *intradot* and *interdot* Coulomb interaction [11] and vanishes only in the limit $d \rightarrow 0$.

Increasing the vertical magnetic field effectively leads to a stronger lateral confinement of the electrons and hence to an increase of the Coulomb energy. Additionally intradot interaction increases faster with increasing magnetic field than the interdot-interaction, that is limited to $1/d$ [9]. This different scaling causes magnetic field dependent correlations in the eigenstates. We show that this can lead to a ground state crossing to fixed M, S, S_z for symmetric DQD and charge polarization in slightly asymmetric dots.

To take correlations into account we compute the eigenstates and the corresponding eigenenergies by numerically diagonalizing the many-body Hamiltonian (3), i.e. we expand the eigenstates in a finite basis of Slater determinants [14].

Calculating the magnetic-field dependence of the energy spectrum for three electrons inside a symmetric DQD to angular momentum $M = -5$ and spin $S = S_z = 3/2$, we find a crossing between the two energetically lowest states as illustrated in Fig. 1. Since the crossing states only differ in parity, the accidental crossing converts into an anticrossing if the parity conservation is broken by a slight asymmetry between the dots leading to two strongly charge-polarized states. For specific parameters the parity crossing and hence the charge-polarization found for this subspace of quantum numbers becomes visible in the ground state (GS) as illustrated in Fig. 2. For other parameters the parity crossing will either arise in excited states or even disappear completely as shown in Fig. 3. The asymmetry between the dots can be either intrinsic or caused by a small bias voltage, as it is applied in transport experiments [15]. We model the asymmetry between the dots by adding the term $\hat{\mathcal{V}}_z = V_z \cdot \hat{\mathcal{I}}_z$ to the Hamiltonian (3) where V_z is the energy difference between upper and lower dot for a single electron. While the ground state is nearly unpolarized for general magnetic field strengths, Fig. 2 shows a strongly polarized ground state at the magnetic field where the anticrossing occurs. The minimal value of $\langle \mathcal{I}_z \rangle = -0.5$ corresponds to two electron charges in the lower dot and one in the upper. Thus we find the astonishing effect that electrons become localized in one of the dots by simply changing the vertical magnetic

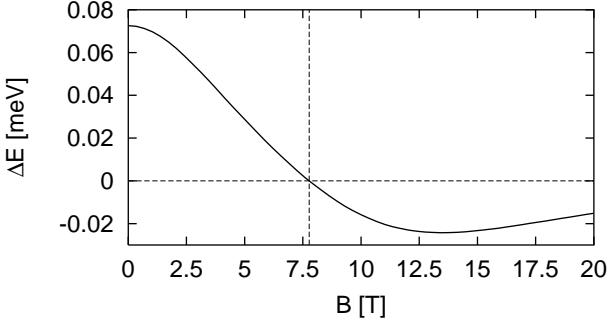


FIG. 1: Energy difference of the lowest two eigenstates to $\hat{\mathcal{H}}$ ($M = -5$ and $S = S_z = 3/2$) as a function of the magnetic field B . $t = -0.059$ meV, $\hbar\omega_0 = 2.96$ meV and $d = 19.6$ nm. The crossing takes place at $B = 7.77$ T (dashed vert. line).

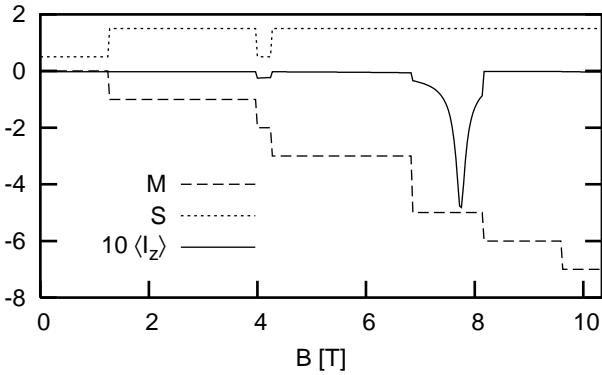


FIG. 2: Angular momentum M , total spin S and expectation value of the z-component of the isospin $\langle \mathcal{I}_z \rangle$ for the three electron ground state to $\hat{\mathcal{H}} + \hat{\mathcal{V}}_z$. $\hat{\mathcal{V}}_z = 5.9 \cdot 10^{-4} \hat{\mathcal{I}}_z$ meV represents a slight asymmetry between the dots. The peak in $\langle \hat{\mathcal{I}}_z \rangle$ illustrates the charge localization that corresponds to the parity crossing (see text). Other parameters are the same as in Fig. 1.

field. It is important to note that the strength of the asymmetry (i.e. V_z) only determines the width of the localization dip in Fig. 2 but even for arbitrarily small asymmetries the ground state is strongly polarized at the anticrossing with $\langle \mathcal{I}_z \rangle = -0.5$. Since $[\hat{\mathcal{L}}_z, \hat{\mathcal{V}}_z] = [\hat{\mathcal{S}}^2, \hat{\mathcal{V}}_z] = [\hat{\mathcal{S}}_z, \hat{\mathcal{V}}_z] = 0$, $\hat{\mathcal{V}}_z$ couples only states with same total angular momentum and total spin. Therefore a similar effect does not occur in the well known ground state crossing between states that differ in M and/or S [9].

In the following we study the reported parity crossing in the GS of a symmetric DQD in more detail. Without tunneling I_z is conserved and since both dots are identical the ground state will be two-fold degenerate with $I_z = \pm 0.5$. Switching on tunneling their degeneracy

is lifted and the GS splits in two non-degenerate parity eigenstates $|P = \pm 1\rangle$ because of their different occupations of symmetric and antisymmetric orbitals. In particular Fig. 1 illustrates that for magnetic fields $B < 7.8$ T $|P = -1\rangle$ is favored by tunneling i.e. it has a higher occupation of symmetric orbitals than $|P = +1\rangle$. However due to magnetic-field dependent correlations the occupation of symmetric orbitals decreases for $|P = -1\rangle$ but increases for $|P = +1\rangle$, so that by increasing the magnetic field finally $|P = +1\rangle$ becomes the GS. Fig. 3 shows the parity as a function of tunneling and external magnetic field for the subspace $M = -5$ and spin $S = S_z = 3/2$. The crossing exists from zero tunneling up to $t \approx 0.27$ meV, which suggests to treat the tunneling t as a small perturbation. For small tunneling (tunneling much smaller than the energy spacing between degenerate ground state and first excited state at $t = 0$) the parity eigenstates are to first order perturbation theory given by $|P = \pm 1\rangle \approx (|I_z = \frac{1}{2}\rangle \pm |I_z = -\frac{1}{2}\rangle)/\sqrt{2}$. and their energy splitting is $2\langle I_z = \frac{1}{2} | \hat{\mathcal{H}}_T | I_z = -\frac{1}{2} \rangle(B)$. As indicated this matrix element depends on the magnetic field due to the magnetic-field dependent correlations present in the states $|I_z = \pm \frac{1}{2}\rangle$. To first order the crossing occurs at $B = 7.85$ T where the matrix element vanishes, and is independent of t in good agreement with the exact results for small tunneling (see Fig. 3). For strong tunneling however higher order effects (coupling to higher states) come into play causing the crossing to disappear for $t > 0.27$ meV. Breaking the vertical symmetry of the DQD the two parity eigenstates are coupled and the parity-crossing converts into an anti-crossing, thereby lifting their accidental degeneracy by an amount V_z . At the anticrossing the eigenstates are approximately given by $I_z = \pm \frac{1}{2}$ and are thus strongly charge polarized. We want to note that the parity-crossing and the related strong charge-polarization is not restricted to the total angular momentum and total spin chosen here but also occurs for other sets of quantum numbers. Furthermore a symmetric DQD containing any odd number of electrons has a degenerate ground state at $t = 0$ and similar parity crossings are expected for higher odd numbers of electrons in the DQD (the ground state of an even number of electrons at $t = 0$ has $I_z = 0$ and is non-degenerate).

The polarization of the three-electron GS can be detected in a transport experiment through the DQD [7, 8, 15, 16]. If a small transport voltage, V_{SD} , accross the DQD is applied [17] at constant magnetic field, the conductance G has a peak structure as a function of the gate voltage. The height of the conductance peaks G^{peak} corresponding to the transitions between two and three electrons or three and four electrons inside the DQD are shown

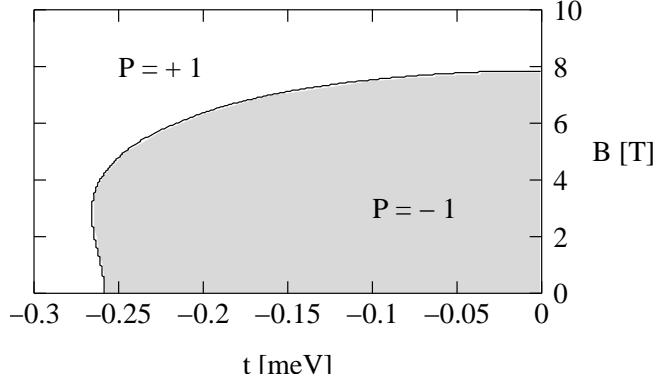


FIG. 3: Dependence of the parity P for angular momentum $M = -5$ and $S = 3/2$ on magnetic field B and tunneling t . The solid line indicates where the crossing between the parity eigenstates takes place. Other parameters are the same as in Fig. 1.

as a function of the magnetic field and for two different temperatures in Fig. 4. A comparison with Fig. 2 shows that the current through the DQD is suppressed at the magnetic field, where the three-electron GS becomes polarized. We want to point out that since the asymmetry between the dots is weak only the two lowest three-electron states are polarized (in opposite direction) whereas the other states and in particular the two and four electron ground states are unpolarized (in contrast to Ref. [8]). In our calculations we assume that transport is described by sequential tunneling processes in and out of the many-particle eigenstates of the isolated DQD. This is a good approximation for weak tunnel contacts between the reservoirs and the DQD, i.e. the tunneling strength to the external reservoirs is smaller than the interdot tunneling and the finite lifetime broadening of the DQD states is smaller than temperature [18]. For the tunneling events a transition rate can be calculated, which we call T^+ (T^-) for a transition caused by a tunneling event through the upper (lower) barrier. In the following we discuss the transition between two and three electrons in the dot, but the arguments are equally valid also for the next conductance peak.

Assuming that an electron in the upper (lower) reservoir can only tunnel into the upper (lower) dot, the transition rate T^+ between a two particle state and a three particle state is proportional to the spectral weight $T_{N_e=3 \rightarrow N_e=2}^+ \propto \sum_{n,m,\sigma} |\langle N_e = 2 | d_{nm+\sigma} | N_e = 3 \rangle|^2$ [19], where $d_{nm+\sigma}$ denotes the annihilation operator for the orbital $|nm + \sigma\rangle$ in the upper dot [14], similarly $T_{N_e=3 \rightarrow N_e=2}^- \propto \sum_{n,m,\sigma} |\langle N_e = 2 | d_{nm-\sigma} | N_e = 3 \rangle|^2$. Due to the small transport voltage only the two transport channels that include the unpolarized two-electron GS and one

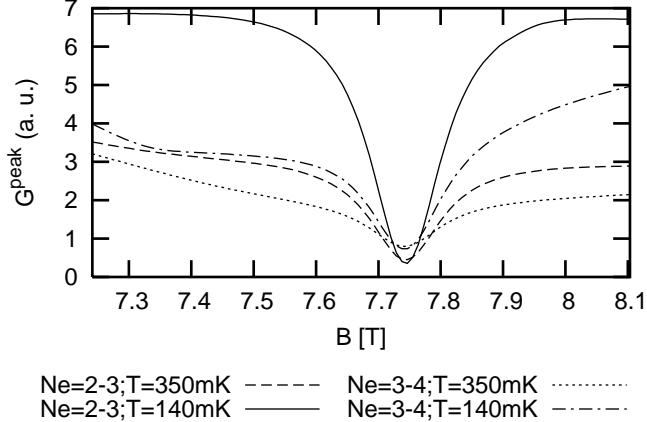


FIG. 4: Calculated height of third and fourth conductance peak (transition from $N_e = 2$ to $N_e = 3$ or from $N_e = 3$ to $N_e = 4$) as a function of the magnetic field for two temperatures. Parameters: $V_{sd} = 12\mu\text{V}$; $T = 140$ mK. Other parameters are the same as in Fig. 1 and 2. In particular the asymmetry between the lower and upper dot $V_z = 10^{-2}|t| \approx 0.6\mu\text{eV}$.

of the polarized three-electron states (GS and first excited state) lie within the transport window. Higher channels only contribute due to the finite temperature and can be further suppressed by lowering the temperature. For both transport channels that include polarized three-electron states one of the transition rates either for the tunneling in or tunneling out process is isospin-blocked. T^- (T^+) is suppressed, if the three electron state has two electrons localized in the upper (lower) dot. For a current to flow through the DQD both tunneling processes are necessary, which is expressed by the effective tunneling rate $\Gamma \propto \frac{T^- T^+}{T^- + T^+}$ [20]. Therefore the current is strongly reduced due to an isospin blockade of both channels. Away from the crossing the three-electron states are no longer polarized so that the transition through both barriers is possible.

We conclude: Magnetic-field dependent Coulomb correlations affect the eigenstates' tunneling energies differently depending on their parity leading to additional magnetic-field induced level-crossings between states with different parity but same angular momentum and spin in a perfectly symmetric DQD. The magnetic-field dependent charge-polarization in symmetry-broken DQDs is due to an anticrossing of two eigenstates with different parity. The charge polarization takes also place in the ground state and is detectable in a transport experiment through the DQD as it leads to an isospin blockade at the magnetic field where the polarization occurs. The resulting polarized eigenstates $|\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ can be seen as a

qubit which can be switched by the applied bias voltage. A controlled superposition of the two states can then be achieved by adjusting the magnetic field. The parity crossing and the related magnetic-field dependent charge polarization appear also for an odd number of electrons greater than three and in different subsets of quantum numbers.

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* Electronic address: david.jacob@ua.es

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